§21. Molecular Dynamics Study of Strongly-Coupled Coulomb Polymers

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A strongly coupled Coulomb system is one of the important areas of plasma and statistical physics, which is realized by either compressing materials to Angstrom ranges or by cooling them to very low temperature. The strongly coupled system is found in condensed matters, highly compressed laser-irradiated plasmas, the stellar interiors [1], and even in live organisms like nucleic acids and DNA [2]. Under these circumstances, the Coulomb interactions act to organize the structure of matters and determine their equilibrium properties. The charged chains of monomers studied here model the *polyampholyte* which consists of the chains of charged monomers (molecular groups) of random sequence [2].

We showed in 1996-97 an existence of three temperature regimes in the phase of the polyampholytes, and a hysteresis against slow changes in temperature for *single-chain polyampholytes* submerged in immobile viscous medium using the molecular dynamics simulations [3]. Following this study, we are investigating the dynamics and equilibrium of multichain polyampholytes which have more freedom than the single-chain case. The equations of motion for the N monomers are,

$$m\frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{LR}(\mathbf{r}_i) - \frac{3T}{a^2}(2\mathbf{r}_i - \mathbf{r}_{i+1} - \mathbf{r}_{i-1}) + \mathbf{F}_{th} - \nu m\mathbf{v}_i, \quad (1)$$

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i. \quad (2)$$

The electrostatic Coulomb force, which is a long-range force, is given by

$$\mathbf{F}_{LR}(\mathbf{r}_i) = \sum_j \frac{Z_i Z_j e^2}{\epsilon|\mathbf{r}_i - \mathbf{r}_j|^2}\hat{\mathbf{r}}_{ij}. \quad (3)$$

When temperature is high $\Gamma = e^2/\epsilon a T < 1$, we have separated chains each of which is a Gaussian coil, as shown in Fig.1(a). Thus, the multichain charged polymers are much less compact than the single-chain polymers. At low temperature such that $\Gamma > 1$, a compact and dense globule is obtained (Fig.1(c)) which results from a collapse of the chains under strong attraction by the Coulomb force. This globule in which the chains are folded and confined is similar to that made of a single chain polyampholyte.

Because of the structure mentioned above, the size of multichain polymers is much more sensitive to temperature of surrounding medium, as shown in Fig.2. The scaling of the gyration radius is $R_{g,sys} \sim T^{1/2} - T^1$, which is steeper than the scaling $R_g \sim T^{1/3}$ for a single chain polyampholyte.

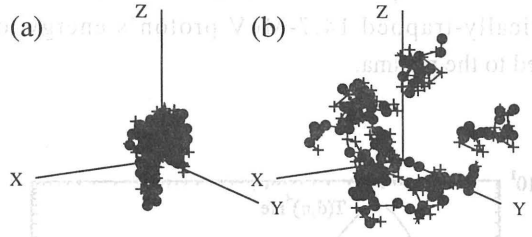

Fig.1 Equilibrium of the multichain polymers, (a) $T < T_0$ and (b) $T > T_0$.

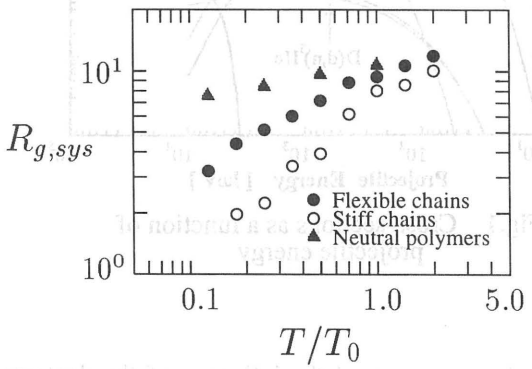

Fig.2 Temperature dependence of the polymer size – gyration radius $R_{g,sys}$.

References

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